Tracing maturity differences in catagenesis stage disperse organic matter using Raman spectroscopy

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The examination and reconstruction of thermal history in sedimentary basins is a widely used and essential discipline of geology. Numerical parameters for the reconstruction of basin evolution can be acquisited by several methods (e.g. vitrinite-reflectance analysis, fluid inclusions microthermometry, etc.). Based on numerous researches and articles, the application of Raman spectroscopy might be a possible and admissible way to determine the development of the thermal history trough the measurement of organic matter (OM) if it is in the metagenesis stage. Based on the previous studies, however, the measurement of diagenesis or catagenesis stage OM is more complicated because of the sensitivity of OM.

The sensitivity of OM comes from the process of biochemical and geochemical gelification that causes structural changes in the OM. With the formation of hydrocarbon the chemical composition changes constantly.

The applicability of Raman spectroscopy in maturity characterization is based on the changes of the structure of OM during the thermal maturation, which is in connection with the appearance, disappearance and change of different Raman active vibration modes during the processes. The principle of the maturity estimation is the following: the OM starts to be ordered with increasing maturity thus the area of disordered peaks on Raman spectra (Fig. 1.) decreases until the graphitic stage where only one peak at 1578 $cm^{-1}$is detectable. The Raman spectra of organic matter, except graphite, can contain first order - G band (1580 - 1600 cm^{-1}); D bands (which vary between 1100 and 1500 cm^{-1}) and second order bands (2450, 2700, 2900 and 3100 cm^{-1}). The peak position, area and full width at half maximum (FWHM) of the maturity the D1 band, that is the most easily detectable D and G peaks change with maturity. With increasing on Raman spectra, shifts towards lower wavenumber, the G band approaches to the graphitic position and the area and FWHM ratio (D1/G) decreases.

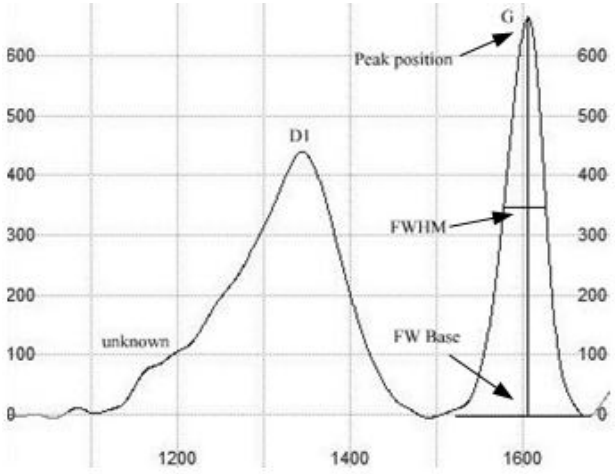

Fig 1.: Raman spectrum of disperse OM between 1000 and 1800 cm^{-1}

The present study inspects the possibility of application of the Raman spectroscopy for determination and identification of thermal history of OM situated in catagenesis stage. Raman analyses were performed on micrometer-sized disperse OM on 21 samples from different depths of a given core. The maturity of all of the samples is in catagenesis stage based on preliminary vitrinite - reflectance measurements. Based on visual kerogene analyses, the kerogen consists of type II and type III OM. The change of the FWHM ratio, integrated area and base width of G and D1 and their peak positions were calculated with the application of software PeakFit. The measurements were executed by Thermo DXR Raman Microscope.